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Fermi surface topology effect on interlayer magnetoresistance with in-plane magnetic field in layered multiband system: Application to FeAs-based superconductors

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Abstract

We propose interlayer magnetoresistance experiments which provide information about Fermi surface topology in layered multiband systems. The interlayer magnetoresistance shows an oscillating behavior with respect to the azimuthal angle of the applied in-plane magnetic field if the Fermi surface is anisotropic. We discuss applications to LaFeAsO, a parent compound of FeAs-based superconductors. We show the results on the paramagnetic state and the antiferromagnetic state based on a mean field calculation.

Key words: iron-pnictide superconductors, Fermi surface topology, interlayer magnetoresistance
71.18.+y, 72.10.-d, 75.47.-m

1. Introduction

FeAs-based layered superconductors have attracted much interest since the discovery [1]. As a basic electronic property the Fermi surfaces have been studied theoretically and experimentally. First principles calculations [2, 3] suggest that the Fermi surface of LaFeAsO consists of hole Fermi surfaces around Γ point and electron Fermi surfaces around M point. The Fermi surfaces measured by ARPES [4, 5, 6, 7, 8] are mostly consistent with this picture, though the measured samples are limited. For example, a single hole pocket and a single electron pocket were observed in $NdFeAsO_{0.9}F_{0.1}$.[7, 8], while the other Fermi pockets predicted by the band calculations were not observed. The hole Fermi surfaces and the electron Fermi surfaces have instability of a magnetic order associated with a nesting of (π,π) wavevector. The magnetically ordered state is a collinear antiferromagnetic state as suggested from the neutron scattering experiments.[9, 10] Quantum oscillation measurements were carried out for magnetic states of a few Fe-based superconductors.[11, 12, 13] Possible folding of Brillouin zone are discussed so that the observed oscillation periods are reproduced.

In this note, we propose an experiment to study Fermi surface topology using the inter-layer magnetoresistance. Our formula is based on an extension of the formula for single-band systems [14, 15, 16] to multi-band systems. We apply the formula to the paramagnetic state and the magnetic state of LaFeAsO. We use the five band model of Ref.[17]. The magnetic state is obtained by a mean field calculation.[18] The interaction term is

$$\begin{aligned} H_{\rm int} &= U\sum_{j,\mu} n_{j\mu\uparrow}n_{j\mu\downarrow} + (U-2J)\sum_{j,\mu<\nu} n_{j\mu}n_{j\nu} \\ &\quad + J\sum_{j,\mu<\nu,\alpha,\beta=\uparrow,\downarrow} d^\dagger_{j\mu\alpha}d^\dagger_{j\nu\beta}d_{j\mu\beta}d_{j\nu\alpha} \\ &\quad + J\sum_{j,\mu<\nu}\left(d^\dagger_{j\mu\uparrow}d^\dagger_{j\mu\downarrow}d_{j\nu\downarrow}d_{j\nu\uparrow} + h.c.\right), \end{aligned} \tag{1}$$

where μ,ν label the five d-orbitals. The operator $d^\dagger_{j\mu\alpha}$ creates an μ-th orbital electron with spin α at j-th site. The number operators are given by $n_{j\mu\alpha} = d^\dagger_{j\mu\alpha}d_{j\mu\alpha}$ and $n_{j\mu} = n_{j\mu\uparrow} + n_{j\mu\downarrow}$. According to Ref.[18], we paramegtrize the interaction terms using U and J. We take $U = 1.4$eV for the inter- and intra-orbital Coulomb interaction parameters and $J = 0.3$eV for the Hund's coupling and the interorbital pair hopping parameters. (A similar calculation using first principles results was given in Ref.[19].)

The inter-layer magnetoresistance formula is derived using a Kubo formula.[19] At zero temperature, the interlayer conductivity is given by

$$\begin{aligned} \sigma_{zz} &= \frac{e^2}{2\pi}\left(\frac{t_c a_c}{\hbar}\right)^2 N_z \sum_\nu \int_{E^{(\nu)}_{\mathbf{k}}=E_F} d\ell_{\mathbf{k}} \frac{1}{\left|v^{(\nu)}_{\mathbf{k}}\right|} \\ &\quad \times \frac{\Gamma/\pi}{\left(\frac{ea_c}{c\hbar}\frac{\partial E^{(\nu)}_{\mathbf{k}}}{\partial \mathbf{k}} \times \mathbf{B}\right)^2 + \Gamma^2}, \end{aligned} \tag{2}$$

where the magnetic field $\mathbf{B} = (B_x, B_y, 0) = B(\cos\phi, \sin\phi, 0)$ is assumed to be in the plane. The coefficient includes the interlayer hopping parameter t_c, the lattice constant in the z-axis, a_c, and the number of layers, N_z. The integration is taken along each Fermi surface given by $E^{(\nu)}_{\mathbf{k}} = E_F$ with $E^{(\nu)}_{\mathbf{k}}$ the energy dispersion of ν-th band. The effect of scattering upon interlayer hopping processes is included by the parameter Γ.

The Fermi surface calculated by the five band model [17] in the paramagnetic phase is shown in Fig.1(a). Figure 1(b) shows the Fermi surface of the collinear antiferromagnetic state. The interlayer magnetoresistance is calculated for both cases as shown in Fig.2. Oscillations are associated with anisotropies in Fermi pockets. Flat regions of the Fermi surfaces primary

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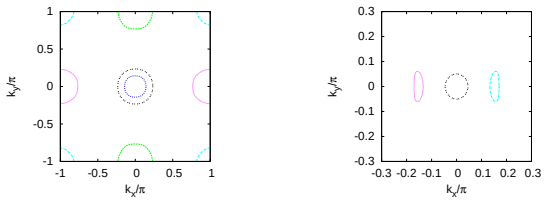
contribute to σ_{zz}. Oscillating behavior is more ponounced for the collinear antiferromagnetic state than for the paramagenetic state. In the paramagnetic state, the Fermi surfaces around $(\pi, 0)$ and $(0, \pi)$ give rise to the oscillation in the interlayer magnetoresistance. In the antiferromagnetic state, the Fermi surface consists of three pockets. Oscillation in the interlayer magnetoresistance mainly associated with the Fermi surfaces around $(\pm 0.15\pi, 0)$. Since the hole Fermi surface around (π, π) is circular, this Fermi surface does not contribute to the interlayer magnetoresistance in both cases. Results based on first principles calculations [19] are consistent with the above results.



(a) (b)

Figure 1: The Fermi surface of the paramagnetic state (a) and the collinear antiferromagnetic state (b).

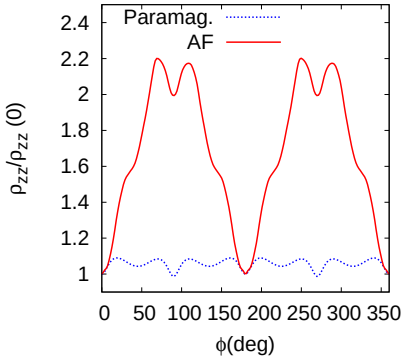


Figure 2: The normalized interlayer magnetoresistances for the paramagnetic state and the collinear antiferromagnetic state. We took $B = 10$T and $\Gamma = 1.0 \times 10^{-4}$eV.

Note that the characteristic energy for the change of the Fermi surface topology is the Fermi energy. Therefore, the temperature effect on the Fermi surface shape is negligible as long as the temperature is much lower than the Fermi energy. However, the temperature effect on the scattering would be important for high temperature.

Information about the scattering effect on the Fermi pockets contributing to the oscillations in ρ_{zz} is extracted from the magnetic field dependence of the peaks in Fig.2. From comparisons of experiments and calculation results one can evaluate the scattering parameter Γ.

Now we comment on the interlayer coupling. The energy dispersion along the z axis is not included in the above calculation. To see the interlayer coupling effect, let us consider the electron band dispersion along the z axis, $\epsilon_k^{(c)} = -2t_c \cos k_z$. Since the Fermi surface topology change is characterized by the Fermi energy, the result would change if t_c larger than or comparable to the Fermi energy. For t_c much less than the Fermi energy, the interlayer coupling effect is negligible.

For Fe-based superconductors with strong three dimensionality, we need to sum over the results at each k_z. If the interlayer hopping is approximated by a simple model, one may apply the Shockley's tube-integral formula [20] to analyze the angle-dependent magnetoresistance oscillations. The angle-dependent magnetoresistance peaks are connected with the vanishing of the electronic group velocity perpendicular to the layers. [21] Since the vanishing condition depends on the Fermi wave-vector, which is azimuthal angle dependent, it is possible to extract further information about the Fermi surface topology.[22]

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